Partition function zeros of the $Q$-state Potts model for non-integer $Q$

Seung-Yeon Kim$^a$, Richard J. Creswick$^{a,*}$, Chi-Ning Chen$^b$, Chin-Kun Hu$^b$

$^a$Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208, USA
$^b$Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan

Abstract

The distribution of the zeros of the partition function in the complex temperature plane (Fisher zeros) of the two-dimensional $Q$-state Potts model is studied for non-integer $Q$. On $L \times L$ self-dual lattices studied ($L \leq 8$), no Fisher zero lies on the unit circle $p_0 = e^{i\theta}$ in the complex $p = (e^{\beta J} - 1)/\sqrt{Q}$ plane for $Q < 1$, while some of the Fisher zeros lie on the unit circle for $Q > 1$ and the number of such zeros increases with increasing $Q$. The ferromagnetic and antiferromagnetic properties of the Potts model are investigated using the distribution of the Fisher zeros. For the Potts ferromagnet we verify the den Nijs formula for the thermal exponent $y_t$. For the Potts antiferromagnet we also verify the Baxter conjecture for the critical temperature and present new results for the thermal exponents in the range $0 < Q < 3$. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The $Q$-state Potts model [1] on a lattice $G$ for integer $Q$ is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j),$$

where $J$ is the coupling constant, $\langle i,j \rangle$ indicates a sum over nearest-neighbor pairs, and $\sigma_i = 1, \ldots, Q$. Fortuin and Kasteleyn [2] have shown that the partition function can be written as

$$Z = \sum_{G' \subseteq G} Q^{n(G')}(e^{\beta J} - 1)^{h(G')},$$

*Corresponding author.
E-mail addresses: kim@cosmos.psc.sc.edu (S.-Y. Kim), creswick.rj@sc.edu (R.J. Creswick)

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Fig. 1. Fisher zeros in the complex $p$ plane of $8 \times 8$ $Q$-state Potts models for (a) $Q = 0.1$ and 0.9, (b) 1.1 and 1.9, (c) 2.1 and 2.9, and (d) 9999.9. In (b) and (c) two unit circles are the locus of the Fisher zeros for the Ising model in the thermodynamic limit.

where the summation is taken over all subgraphs $G' \subseteq G$, and $n(G')$ and $b(G')$ are, respectively, the number of clusters and occupied bonds in $G'$. In Eq. (2) $Q$ need not be an integer and Eq. (2) defines the partition function of the $Q$-state Potts model for non-integer $Q$. In this paper we discuss the ferromagnetic (FM) and antiferromagnetic (AF) properties of the two-dimensional Potts model for non-integer $Q$ using the partition function zeros in the complex temperature plane (Fisher zeros).

We have calculated the exact partition function of the Potts model on finite lattices of size $3 \leq L \leq 8$ by the Chen–Hu algorithm [3] based on the Fortuin–Kasteleyn representation. We have used self-dual boundary conditions [4] for which the Fisher zeros of the Potts model map into themselves under the duality transformation, $p \rightarrow 1/p$. 
where \( p = (e^{i\theta} - 1)/\sqrt{Q} \). The self-dual lattices considered in this paper are periodic in the horizontal direction and there is another site above the \( L \times L \) square lattice, which connects to \( L \) sites on the first row.

Fig. 1 shows the Fisher zeros in the complex \( p \) plane of the Potts model for several values of non-integer \( Q \). For \( Q < 1 \) no zero lies on the unit circle \( p_0 = e^{i\theta} \) and as \( Q \) approaches one from below some zeros approach the unit circle. In Fig. 1a, we have omitted half of the Fisher zeros which give no more information because they can be obtained using the duality transformation from the Fisher zeros in the figure. For \( Q > 1 \) zeros begin to lie on the unit circle \( p_0 \) and the number of zeros on the unit circle increases with increasing \( Q \). Fig. 1b shows the Fisher zeros in the range \( 1 < Q < 2 \). The two circles shown are the FM and AF loci for the 2-state (Ising) model in the thermodynamic limit [5]. For \( Q > 2 \) the zeros in the AF region (Re(\( p \)) < 0) become more scattered. Finally, as shown in Fig. 1d, for large \( Q \) all the zeros lie on the unit circle \( p_0 \) [4]. The distribution of zeros varies continuously with \( Q \) with the exception of \( Q = 1 \) and \( Q = 2 \). For \( Q = 1 \) the zeros are all degenerate at \( p = -1 \) [4], while for \( Q = 2 \) the symmetry between the FM and AFM Ising model forces the AF zeros to lie on the locus \( p = -\sqrt{2} + e^{i\theta} \).

2. The ferromagnetic Potts model

There is no rigorous proof that the FM critical point \( p_c = 1 \) for \( Q < 4 \) except for \( Q = 2 \) [1]. For \( 1 < Q < 4 \) we observe that the zero closest to the positive real axis always lies on the unit circle and approaches the critical point \( p_c = 1 \) in the thermodynamic limit. For \( Q < 1 \), however, because no zero lies on the unit circle for a finite-size lattice, we need to calculate the FM critical point from the zero closest to the point \( p_c = 1 \) (the first zero). By using the Bulirsch–Stoer (BST) algorithm [6,7] we extrapolated our results for finite lattices to infinite size. The error estimates are twice the difference between the \((n-1,1)\) and \((n-1,2)\) approximants. We find that the first zero converges on the critical point \( p_c = 1 \).

From the first zero, \( p_1 \), we have calculated the thermal exponent \( y_t(L) \) defined as [8]

\[
y_t(L) = -\frac{\ln[\text{Abs}[p_1(L + 1)]/\text{Abs}[p_1(L) - 1]]}{\ln[(L + 1)/L]}
\]

or

\[
y_t(L) = -\frac{\ln[\text{Im}[p_1(L + 1)]/\text{Im}[p_1(L)]]}{\ln[(L + 1)/L]}
\]

For \( Q < 1 \), the imaginary part of the first zero is not a monotonic function of \( L \), and so in this range we used Eq. (3) to calculate \( y_t \). For \( Q > 1 \) Eq. (4) was found to give the best estimate. Fig. 2 shows the BST estimates of the thermal exponent which are in excellent agreement with the den Nijs formula \( y_t = (3 - 3\alpha)/(2 - \alpha) \) [9], where
Fig. 2. The thermal exponent $y_t$ of the Potts ferromagnet by the BST estimates (filled circles) and by the den Nijs formula (continuous curve).

Table 1
The real part Re($p_a$) and the imaginary part Im($p_a$) of the zero $p_a(L)$ closest to the antiferromagnetic interval for $Q = 0.1$ and $2.9$. The last row is the BST extrapolation to infinite size.

<table>
<thead>
<tr>
<th>$Q$</th>
<th>L</th>
<th>Re($p_a$)</th>
<th>Im($p_a$)</th>
<th>2.9</th>
<th>Re($p_a$)</th>
<th>Im($p_a$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>4</td>
<td>$-0.0902065$</td>
<td>$0.00855442$</td>
<td></td>
<td>$-0.501335$</td>
<td>$0.198694$</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>$-0.0844057$</td>
<td>$0.00443054$</td>
<td></td>
<td>$-0.507772$</td>
<td>$0.137197$</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>$-0.0823869$</td>
<td>$0.00272837$</td>
<td></td>
<td>$-0.511662$</td>
<td>$0.107013$</td>
</tr>
<tr>
<td>$\infty$</td>
<td>$-0.078(4)$</td>
<td>$-0.001(2)$</td>
<td></td>
<td>$-0.527(5)$</td>
<td>$0.019(41)$</td>
<td></td>
</tr>
<tr>
<td>Baxter’s conjecture</td>
<td></td>
<td>$-0.07956$</td>
<td>$0$</td>
<td></td>
<td>$-0.5586$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

$x = (2/\pi)\cos^{-1}(\sqrt{Q}/2)$. Blöte et al. [10] have obtained results similar to Fig. 2 using heat capacity data on infinitely long strips.

3. The antiferromagnetic Potts model

For AF interaction $J < 0$ the physical interval is $0 \leq \theta J \leq 1$, which corresponds to $-1/\sqrt{Q} \leq p \leq 0$. Baxter [11] has conjectured the existence of an AF critical point for $Q \leq 3$ at $p_c = (\sqrt{4 - Q} - 2)/\sqrt{Q}$, and we expect that in the thermodynamic limit the locus of the Fisher zeros cuts the negative real axis between $-1/\sqrt{Q}$ and 0. For $Q = 2.9$ and $L = 8$ (Fig. 1c) two zeros already lie on the negative real axis, but they are outside the physical interval. Table 1 shows the real and imaginary parts of the zero $p_a(L)$ closest to the AF interval of the negative real axis for $Q = 0.1$ and $2.9$ for even-size lattices, and in Table 1 the last row are the BST estimates for $L \to \infty$. Fig. 3 shows the BST estimates of the critical points of the Potts antiferromagnet from the Fisher zeros for $0 < Q < 3$ which are in excellent agreement with the Baxter conjecture [11].
Fig. 3. The critical point of the Potts antiferromagnet by the BST estimates (filled circles) and by the Baxter conjecture (continuous curve).

Fig. 4. The thermal exponent $y_t(L)$ of the Potts antiferromagnet as a function of $Q$ for $L = 4$ and 6. Note the large finite-size effect as $Q$ approaches 3.

From the Fisher zeros we have also calculated the thermal exponent $y_t(L)$ defined as

$$y_t(L) = \frac{-\ln\{|\text{Abs}[p_a(L + 2) - p_c]/\text{Abs}[p_a(L) - p_c]|\}}{\ln[(L + 2)/L]}.$$  (5)

Fig. 4 shows the thermal exponent $y_t(L)$ for $0 < Q < 3$. In Fig. 4 as $Q$ increases the thermal exponent decreases and around $Q = 2$ it is consistent with the known exact value $y_t = 1$ of the Ising model. Note that these data are calculated from lattices of size $L = 4$, 6, and 8 only, and no attempt is made to extrapolate to infinite size.

To our knowledge these are the first such calculations of $y_t$ for non-integer $Q$. Of course for the Ising model, $Q = 2$, the exact result $y_t = 1$ has been known for many years, and our results are consistent with this. The value of $y_t$ for $Q = 3$ has been the subject of some debate recently. Ferreira and Sokal [12,13] expect $y_t = \frac{1}{2}$, while Wang et al. [14,15] found $y_t = 0.77$. Although it might appear from Fig. 4 that our results for $Q = 3$ agree with the result of Wang et al., we must emphasize that these
results are for very small lattices and have not been extrapolated to infinite size. If we include calculations for \( Q = 3 \) using the microcanonical transfer matrix [7] for \( L = 10 \), and apply the BST algorithm our results are inconclusive. We are currently extending our calculations to larger lattices in order to address this interesting question.

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References